REPORT DOCUMENTATION PAGE

Form Approved
OMB No. 0704-0188

1. REPORT DATE *(DD-MM-YYYY)*
04-01-2006

REPRINT

4. TITLE AND SUBTITLE
ENTROPIC LATTICE BOLTZMANN MODEL FOR BURGERS'S EQUATION

5a. CONTRACT NUMBER

5b. GRANT NUMBER

5c. PROGRAM ELEMENT NUMBER
61102F

6. AUTHOR(S)
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5d. PROJECT NUMBER
2304

5e. TASK NUMBER
0T

5f. WORK UNIT NUMBER
B1

7. PERFORMING ORGANIZATION NAME(S) AND ADDRESS(ES)
Air Force Research Laboratory/VSBYA
29 Randolph Road
Hanscom AFB MA 01731-3010

8. PERFORMING ORGANIZATION REPORT NUMBER
AFRL-VS-HA-TR-2005-1201

9. SPONSORING / MONITORING AGENCY NAME(S) AND ADDRESS(ES)

10. SPONSOR/MONITOR'S ACRONYM(S)

11. SPONSOR/MONITOR'S REPORT NUMBER(S)

12. DISTRIBUTION / AVAILABILITY STATEMENT
Approved for Public Release; Distribution Unlimited.

*Dept Math, Tufts University, Medford, MA

13. SUPPLEMENTARY NOTES
REPRINTED FROM: PHIL. TRANS. R. SOC. LOND. A, Vol 362, pp 1691-1701, 2004.

14. ABSTRACT

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15. SUBJECT TERM:
Lattice Boltzmann Bergers's equation
Kintic theory

16. SECURITY CLASSIFICATION OF:			17. LIMITATION OF ABSTRACT	18. NUMBER OF PAGES	19a. NAME OF RESPONSIBLE PERSON
a. REPORT		c. THIS PAGE			Jeffrey Yepez
UNCLAS	UNCLAS	UNCLAS	SAR		19b. TELEPHONE NUMBER *(include area code)* 781-377-5957

10.1098/rsta.2004.1410

THE ROYAL SOCIETY

Entropic lattice Boltzmann model for Burgers's equation

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Published online 28 May 2004

Entropic lattice Boltzmann models are discrete-velocity models of hydrodynamics that possess a Lyapunov function. This feature makes them useful as nonlinearly stable numerical methods for integrating hydrodynamic equations. Over the last few years, such models have been successfully developed for the Navier–Stokes equations in two and three dimensions, and have been proposed as a new category of subgrid model of turbulence. In the present work we develop an entropic lattice Boltzmann model for Burgers's equation in one spatial dimension. In addition to its pedagogical value as a simple example of such a model, our result is actually a very effective way to simulate Burgers's equation in one dimension. At moderate to high values of viscosity, we confirm that it exhibits no trace of instability. At very small values of viscosity, however, we report the existence of oscillations of bounded amplitude in the vicinity of the shock, where gradient scale lengths become comparable with the grid size. As the viscosity decreases, the amplitude at which these oscillations saturate tends to increase. This indicates that, in spite of their nonlinear stability, entropic lattice Boltzmann models may become inaccurate when the ratio of gradient scale length to grid spacing becomes too small. Similar inaccuracies may limit the utility of the entropic lattice Boltzmann paradigm as a subgrid model of Navier–Stokes turbulence.

Keywords: lattice Boltzmann; Burgers's equation; kinetic theory

1. Introduction

Lattice Boltzmann models of hydrodynamics (Benzi *et al.* 1992; Succi 2001) evolve a single-particle distribution function in discrete time-steps on a regular spatial grid. The velocity space is discrete, comprised of (possibly linear combinations of) the lattice vectors themselves. Though this constitutes a drastic truncation of the continuum Boltzmann equation, it has been shown that the derivative hydrodynamic equations may emerge unscathed in the limit of small Knudsen number. It is required only that the kinetic collision operator conserve the desired hydrodynamic quantities, such as mass, momentum and energy, and that the lattice possess sufficient symmetry.

One contribution of 21 to a Theme 'Connecting scales: micro, meso and macro processes'.

In recent years it has been shown that these models may also be constructed with a Lyapunov function—a discrete-time and discrete-velocity version of Boltzmann's celebrated H theorem—as is appropriate for a hydrodynamic equation with dissipation. In this case, such models are called *entropic lattice Boltzmann models* (Boghosian *et al.* 2001; Karlin *et al.* 1998, 1999), and it has been proposed that they *may* have two other very desirable features.

(i) First, they may suppress the growth of numerical instabilities, and thereby make the simulation nonlinearly stable (Ansumali & Karlin 2000, 2002; Boghosian *et al.* 2001) even for arbitrarily small viscosities. This argument is based on the premise that numerical instabilities evolve in ways that would be precluded by the existence of a well-behaved Lyapunov function. The upper limit to the Reynolds numbers attainable by entropic lattice Boltzmann models is therefore determined by loss of resolution of the smallest eddies, rather than by loss of stability.

(ii) More recently, it has been posited that entropic lattice Boltzmann models of the Navier–Stokes equations constitute a natural subgrid model of turbulence (Chen *et al.* 2003). That is, even if the grid spacing is too coarse to resolve the smallest eddies, the evolution of the Lyapunov function is necessarily monotonic, and it is argued that this may accurately model turbulent dissipation at subgrid length-scales.

Most lattice Boltzmann models employ a collision operator of Bhatnagar–Gross–Krook (BGK) form, with collisional relaxation time τ (Qian *et al.* 1992). Since transport coefficients such as viscosity are proportional to the quantity $\tau - \frac{1}{2}$, there is incentive to make τ as small as possible to decrease viscosity and thereby increase Reynolds number. In non-entropic lattice Boltzmann models, stability is guaranteed only for $\tau \geqslant 1$, severely limiting attainable viscosities. In entropic lattice Boltzmann models, by contrast, τ is made a function of the incoming state by solving for the smallest value $\tau^* < 1$ that does not increase H. The value then used is $\tau = \tau^* + \kappa(1 - \tau^*)$, where $0 < \kappa < 1$ is an independent variable. It has been shown that the viscosity will be proportional to κ, and may therefore be made arbitrarily small by the appropriate choice of κ (Boghosian *et al.* 2001; Karlin *et al.* 1998, 1999). In this way, the entropic lattice Boltzmann methodology allows for arbitrarily low viscosity together with a rigorous discrete-time H theorem.

In earlier papers, we constructed entropic lattice Boltzmann models for the incompressible Navier–Stokes equations that are Galilean invariant to second order in Mach number, and we showed that the requirement of Galilean invariance makes the choice of H function unique (Boghosian *et al.* 2003*a*,*b*). More specifically, we showed that the required function has the form of the Burg entropy in two dimensions, and the Tsallis entropy in higher dimensions.

In this work, we construct an entropic lattice Boltzmann model for Burgers's equation. There is pedagogical value in this, since it provides a simple illustration of the construction of such a model. More importantly, however, it provides a simple model with which to test the above hypotheses about entropic lattice Boltzmann models. As with entropic models of the Navier–Stokes equations, we may make the viscosity arbitrarily small, giving rise to shock structures with large gradients. We may thereby test whether or not the Lyapunov function truly precludes the onset of

numerical instability, and we may investigate the utility of the model under extreme conditions when shock widths become comparable with the grid spacing.

2. Representation of the distribution function

In the late 1980s, it was shown (Boghosian & Levermore 1987) that one-dimensional lattice-gas models with a conserved mass, a maximum occupation number per site, and a weak spatial asymmetry—that is, a bias for movement in one direction over the other—would generically give rise to Burgers's equation hydrodynamics. The magnitude of the bias should scale with the grid spacing in the continuum limit. Here we recast this general approach, replacing the particulate lattice-gas model with a single-particle distribution function, and introducing the bias in the H function.

We consider a lattice Boltzmann model on a one-dimensional lattice, with a two-component distribution function. We denote by $N_\pm(x,t)$ the number of particles with velocity ±1 at site x and time t. The mass at position x and time t is then

$$\rho(x,t) = N_+(x,t) + N_-(x,t)$$

and this must be conserved in any collision process. We also define the kinetic degree of freedom,

$$u(x,t) = N_+(x,t) - N_-(x,t),$$

which may be thought of as a non-conserved momentum. Together, ρ and u determine the two components of the distribution function:

$$N_\pm(x,t) = \tfrac{1}{2}(\rho(x,t) \pm u(x,t)). \tag{2.1}$$

We demand that the components of the distribution function be positive and have an upper bound of unity:

$$0 \leqslant N_\pm \leqslant 1.$$

This, in turn, implies bounds on the mass and momentum,

$$0 \leqslant \tfrac{1}{2}(\rho \pm u) \leqslant 1,$$

or

$$\left.\begin{aligned} 0 \leqslant \rho \leqslant 2, \\ \max(-\rho, \rho-2) \leqslant u \leqslant \min(+\rho, 2-\rho). \end{aligned}\right\} \tag{2.2}$$

3. H function and equilibrium

Our definition of the H function must be such as to allow an asymmetry in the collision process. We suppose that the H function is of trace form, and weighted by factors $\alpha_\pm \equiv \frac{1}{2}(1 \pm \alpha)$ to provide the asymmetry,

$$H = \alpha_+ h(N_+) + \alpha_- h(N_-),$$

or

$$H = \frac{1+\alpha}{2} h\left(\frac{\rho+u}{2}\right) + \frac{1-\alpha}{2} h\left(\frac{\rho-u}{2}\right). \tag{3.1}$$

The equilibrium distribution is found by extremizing H with respect to u, while keeping ρ fixed. We have

$$0 = \frac{\partial H}{\partial u} = \frac{1+\alpha}{4} h'\left(\frac{\rho+u}{2}\right) - \frac{1-\alpha}{4} h'\left(\frac{\rho-u}{2}\right). \tag{3.2}$$

Note that if $\alpha = 0$, then this is solved by $u = 0$. Moreover, this equation is invariant under the substitutions $u \to -u$ and $\alpha \to -\alpha$. It follows that u may be expanded as a perturbation series in odd powers of α. To do this, we introduce an expansion parameter ε by making the formal replacement $\alpha \to \varepsilon\alpha$, and expanding in powers of ε; at the end of the calculation, we shall reset ε to unity. We find

$$u^{(\mathrm{eq})} = \varepsilon u^{(\mathrm{eq},1)} + \varepsilon^3 u^{(\mathrm{eq},3)} + \cdots,$$

where

$$u^{(\mathrm{eq},1)} = -2\alpha \frac{h'(\frac{1}{2}\rho)}{h''(\frac{1}{2}\rho)}, \tag{3.3}$$

etc. The equilibrium distribution function is then given by

$$N_\pm^{(\mathrm{eq})} = N_\pm^{(\mathrm{eq},0)} + \varepsilon N_\pm^{(\mathrm{eq},1)} + \varepsilon^2 N_\pm^{(\mathrm{eq},2)} + \cdots,$$

where

$$\begin{aligned} N_\pm^{(\mathrm{eq},0)} &= \tfrac{1}{2}\rho, \\ N_\pm^{(\mathrm{eq},1)} &= \mp\alpha \frac{h'(\frac{1}{2}\rho)}{h''(\frac{1}{2}\rho)}, \\ N_\pm^{(\mathrm{eq},2)} &= 0, \\ &\vdots \end{aligned}$$

4. Collision operator

To perform a collision, we suppose that the incoming values of the mass and velocity are ρ and u. We compute the equilibrium value of the velocity $u^{(\mathrm{eq})}$ for the mass ρ, and then we implement the BGK collision operator by letting the post-collision value of u be

$$u' = u + \frac{1}{\tau}(u^{(\mathrm{eq})} - u). \tag{4.1}$$

We choose

$$\tau = \tau^* + \kappa(1 - \tau^*), \tag{4.2}$$

where $\kappa \in [0, 1]$ is an input parameter that shall be used to control the viscosity, and τ^* is the relaxation time that keeps H fixed; that is

$$H\left(\rho, u + \frac{1}{\tau^*}(u^{(\mathrm{eq})} - u)\right) = H(\rho, u). \tag{4.3}$$

Thus, when $\kappa = 0$, the collision keeps H fixed, and H is a constant of the motion. When $\kappa = 1$, the collision simply replaces the incoming state with the equilibrium. For $0 < \kappa \leqslant 1$, H is a Lyapunov function, always decreasing under the dynamics.

From equations (3.1) and (4.3) we get

$$\frac{1+\alpha}{2}h\left(\frac{\rho+u}{2}+\frac{1}{2\tau^*}(u^{(\mathrm{eq})}-u)\right)+\frac{1-\alpha}{2}h\left(\frac{\rho-u}{2}-\frac{1}{2\tau^*}(u^{(\mathrm{eq})}-u)\right)$$
$$=\frac{1+\alpha}{2}h\left(\frac{\rho+u}{2}\right)+\frac{1-\alpha}{2}h\left(\frac{\rho-u}{2}\right). \quad (4.4)$$

This must be solved numerically for τ^*. Such solution is facilitated by the certainty that there is always a solution $\tau^* \in (\frac{1}{2}, 1)$. Equation (4.1) is then used to get τ, and equation (4.1) then gives the post-collision value of u. Finally, this is used in equation (2.1) to get the post-collision distribution function.

The *linearized collision* process is obtained by expanding equation (4.4), treating α, u and $u^{(\mathrm{eq})}$ as order ε, and simplifying the result with equation (3.3). We find that $\tau^* = \frac{1}{2} + \mathcal{O}(\varepsilon)$, whence

$$\tau = \tfrac{1}{2} + \tfrac{1}{2}\kappa + \mathcal{O}(\varepsilon).$$

Remarkably, this *linearized* value of τ is independent of the incoming state. It will be useful in the Chapman–Enskog analysis presented in the next section.

5. Chapman–Enskog analysis

The lattice BGK equation is

$$N_\pm(x \pm c, t + \Delta t) - N_\pm(x,t) = -\frac{1}{\tau}[N_\pm(x,t) - N_\pm^{(\mathrm{eq})}(x,t)],$$

and this may be rewritten as

$$\left\{1+\tau\left[\exp\left(\Delta t\frac{\partial}{\partial t} \pm c\frac{\partial}{\partial x}\right)-1\right]\right\}N_\pm(x,t) = N_\pm^{(\mathrm{eq})}(x,t),$$

which has the formal solution

$$N_\pm(x,t) = \left\{1+\tau\left[\exp\left(\varepsilon^2\Delta t\frac{\partial}{\partial t} \pm \varepsilon c\frac{\partial}{\partial x}\right)-1\right]\right\}^{-1}\sum_{j=0}^{\infty} N_\pm^{(\mathrm{eq},j)}(x,t)\varepsilon^j.$$

Here we have introduced parabolic ordering with the prescription $\Delta t \to \varepsilon^2\Delta t$ and $c \to \varepsilon c$. The distribution function is thus obtained as an expansion,

$$N_\pm = \sum_{\ell=0}^{\infty} N_\pm^{(\ell)}\varepsilon^\ell,$$

where

$$N_\pm^{(0)} = N_\pm^{(\mathrm{eq},0)},$$
$$N_\pm^{(1)} = N_\pm^{(\mathrm{eq},1)} \mp \tau c\frac{\partial N_\pm^{(\mathrm{eq},0)}}{\partial x},$$
$$N_\pm^{(2)} = N_\pm^{(\mathrm{eq},2)} \mp \tau c\frac{\partial N_\pm^{(\mathrm{eq},1)}}{\partial x} - \tau\left[\Delta t\frac{\partial N_\pm^{(\mathrm{eq},0)}}{\partial t} - (\tau-\tfrac{1}{2})c^2\frac{\partial^2 N_\pm^{(\mathrm{eq},0)}}{\partial x^2}\right],$$
$$\vdots$$

We immediately obtain

$$N_{\pm}^{(0)} = \tfrac{1}{2}\rho,$$

$$N_{\pm}^{(1)} = \mp\alpha\frac{h'(\frac{1}{2}\rho)}{h''(\frac{1}{2}\rho)} \mp \frac{\tau c}{2}\frac{\partial\rho}{\partial x},$$

$$N_{\pm}^{(2)} = \tau c\alpha\frac{\partial}{\partial x}\left[\frac{h'(\frac{1}{2}\rho)}{h''(\frac{1}{2}\rho)}\right] - \frac{\tau}{2}\left[\Delta t\frac{\partial\rho}{\partial t} - (\tau - \tfrac{1}{2})c^2\frac{\partial^2\rho}{\partial x^2}\right]$$

$$= -\frac{\tau c\alpha}{2}\left\{\frac{h'(\frac{1}{2}\rho)h'''(\frac{1}{2}\rho)}{[h''(\frac{1}{2}\rho)]^2} - 1\right\}\frac{\partial\rho}{\partial x} - \frac{\tau}{2}\left[\Delta t\frac{\partial\rho}{\partial t} - \frac{\kappa c^2}{2}\frac{\partial^2\rho}{\partial x^2}\right],$$

$$\vdots$$

where we have used the linearized value of τ in the last step.

Finally, we demand that the higher-order corrections to the distribution function do not alter the definition of the conserved quantity $\rho = N_+ + N_-$. That is, we demand that $N_+^{(j)} + N_-^{(j)} = 0$ for $j \geqslant 1$. We see that this is automatic for $j = 1$, and that for $j = 2$ we get the hydrodynamic equation

$$\frac{\partial\rho}{\partial t} + \frac{c\alpha}{\Delta t}\left\{\frac{h'(\frac{1}{2}\rho)h'''(\frac{1}{2}\rho)}{[h''(\frac{1}{2}\rho)]^2} - 1\right\}\frac{\partial\rho}{\partial x} = \frac{\kappa c^2}{2\Delta t}\frac{\partial^2\rho}{\partial x^2}. \tag{5.1}$$

6. Recovery of Burgers's equation

The hydrodynamic equation obtained in the last section will be of the form of Burgers's equation if we demand that the expression in brackets in equation (5.1) is a linear function of ρ. To this end, we demand

$$\frac{h'(z)h'''(z)}{[h''(z)]^2} - 1 = -2az - b,$$

or

$$\frac{\mathrm{d}}{\mathrm{d}z}\left[\frac{h'(z)}{h''(z)}\right] = 2az + b,$$

where a and b are constants to be chosen later. This integrates to yield

$$\frac{h'(z)}{h''(z)} = az^2 + bz + c,$$

where c is a constant of integration. If we define $g(z) = h'(z)$, this may be written

$$\frac{g'(z)}{g(z)} = \frac{1}{az^2 + bz + c}.$$

It is simplest to choose $a = 1$ and $b = c = 0$, so that this integrates to yield

$$g(z) = \exp(-1/z)$$

to within an arbitrary multiplicative constant. Other choices for b and c are possible, and may yield alternative H functions, but that is outside the scope of the present work. Finally, we integrate one more time to obtain

$$h(z) = z\exp(-1/z) + \mathrm{Ei}(-1/z), \tag{6.1}$$

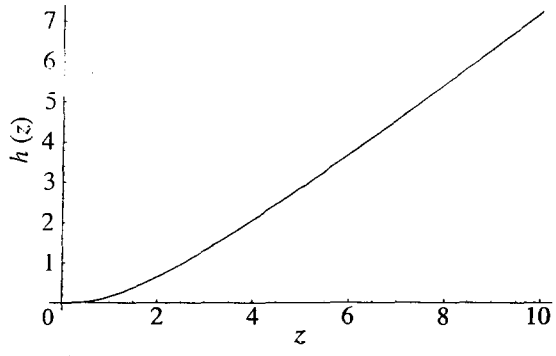

Figure 1. $h(z)$ versus z.

for $z > 0$, where 'Ei' is the exponential integral function. This monotonically increasing and convex function is plotted in figure 1.

Using the form of $h(z)$ derived in equation (6.1), we find that equation (5.1) reduces to

$$\frac{\partial \rho}{\partial t} - \frac{c\alpha}{\Delta t}\rho\frac{\partial \rho}{\partial x} = \frac{\kappa c^2}{2\Delta t}\frac{\partial^2 \rho}{\partial x^2}.$$

If we define the rescaled dependent variable

$$w \equiv -\frac{c\alpha}{\Delta t}\rho,$$

and identify the viscosity,

$$\nu \equiv \frac{\kappa c^2}{2\Delta t},$$

then this simplifies to Burgers's equation:

$$\frac{\partial w}{\partial t} + w\frac{\partial w}{\partial x} = \nu\frac{\partial^2 w}{\partial x^2}.$$

Equation (6.1) for $h(z)$ has the additional virtue of allowing for an analytic solution for the equilibrium distribution. Inserting it into equation (3.2), we have

$$(1+\alpha)\exp\left(\frac{-2}{\rho+u}\right) - (1-\alpha)\exp\left(\frac{-2}{\rho-u}\right) = 0,$$

from which we may solve exactly for the equilibrium value of u:

$$u^{(\mathrm{eq})} = \frac{2}{\ln[(1+\alpha)/(1-\alpha)]}\left[1 - \sqrt{1 + \frac{\rho^2}{4}\left[\ln\left(\frac{1+\alpha}{1-\alpha}\right)\right]^2}\right]. \tag{6.2}$$

7. Implementation

We implemented the above-described entropic lattice Boltzmann model for Burgers's equation on grids of size $N = 64$ and $N = 512$, with initial conditions

$$\rho(x,0) = \rho_0 + \rho_1 \cos\left(\frac{2\pi x}{N}\right).$$

We took $\alpha = -0.1$, $\rho_0 = 0.8$ and $\rho_1 = 0.2$ in both cases. On the $N = 64$ grid we took $\kappa = 0.05$, and on the $N = 512$ grid we took $\kappa = 0.01$. Both of these were intended as extreme cases, designed to test the robustness of the algorithm. The first has a very coarse grid, while the second has a very low viscosity and hence a very narrow shock. In both cases, the ratio of shock width to grid spacing is small.

A *regula falsi* root finder was used to solve for the post-collision velocity, with initial guess $2u^{(\mathrm{eq})} - u$, and precautions were taken so that the iterates never left the feasible region described by the inequality in equation (2.2). Under these circumstances, convergence was very robust. It is likely that performance could be improved by using the *regula falsi* algorithm to get in the vicinity of the solution, and then switching over to a Newton–Raphson solver, but we did not explore this possibility.

Figure 2 shows the $N = 64$ simulation for time increments of 200, from $t = 0$ to $t = 1800$. This is long enough to see the formation, steepening and decay of the shock. By $t = 1000$, it is clear that the advancing shock is leaving small oscillations behind it. These oscillations remain bounded in amplitude, and eventually decay to zero with the shock. While these oscillations are not, strictly speaking, a Gibbs phenomenon—since that would manifest itself both ahead of and behind the shock—they are similar in that their amplitude remains bounded, and goes to zero as the grid is refined for fixed shock width.

Figure 3 shows the $N = 512$ simulation for time increments of 1024, from $t = 0$ to $t = 1800$. Once again, this is long enough to see the formation, steepening and decay of the shock. By $t = 4608$, it is clear that the advancing shock is leaving small oscillations behind it. This oscillatory tail actually grows in length, while remaining bounded in amplitude. Once again, it eventually decays to zero with the shock. In both cases, if the rapid oscillations were filtered out, the remaining smooth component of the solution would match the exact solution of Burgers's equation almost perfectly.

8. Conclusions

We have derived an entropic lattice Boltzmann model for Burgers's equation, and used it to perform a fully explicit, unconditionally stable numerical integration of these equations. The model has the virtue of allowing for an analytic solution of the equilibrium distribution function, though it does require a numerical root-finding procedure in order to implement the collision operator. The form of the H function that is required, presented in equation (6.1), involves the exponential integral function.

We have also used this model to simulate Burgers's equation in one dimension in two extreme situations: the first with an unduly coarse grid, and the second with a very small viscosity. Both situations give rise to small ratios of shock width to grid spacing. In both situations, we noted the presence of oscillations of bounded amplitude trailing the shock, and driven by the strong spatial gradients present there. While the Lyapunov function did indeed prevent the unbounded growth of these oscillations into a full-fledged numerical instability, their presence is nonetheless troubling if one's goal is to use entropic collision operators as subgrid models of turbulence. Subgrid turbulence models endeavour to do exactly what we have done in the simulations described herein: they use a grid spacing that is known to be too large to resolve the gradient scale lengths present, and argue that the effect of

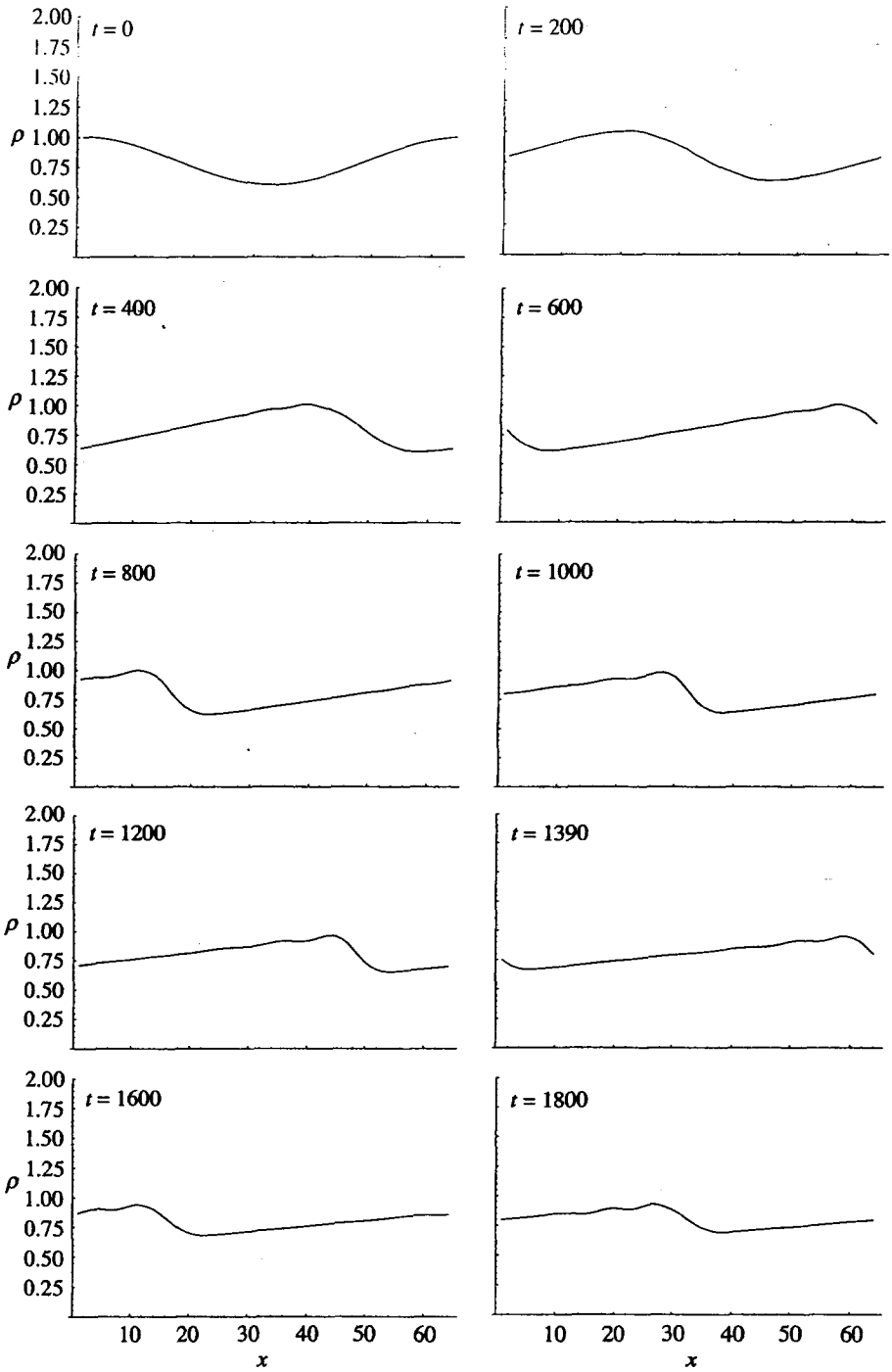

Figure 2. $\rho(x,t)$ versus x for a sequence of times t for $N = 64$ and $\kappa = 0.05$.

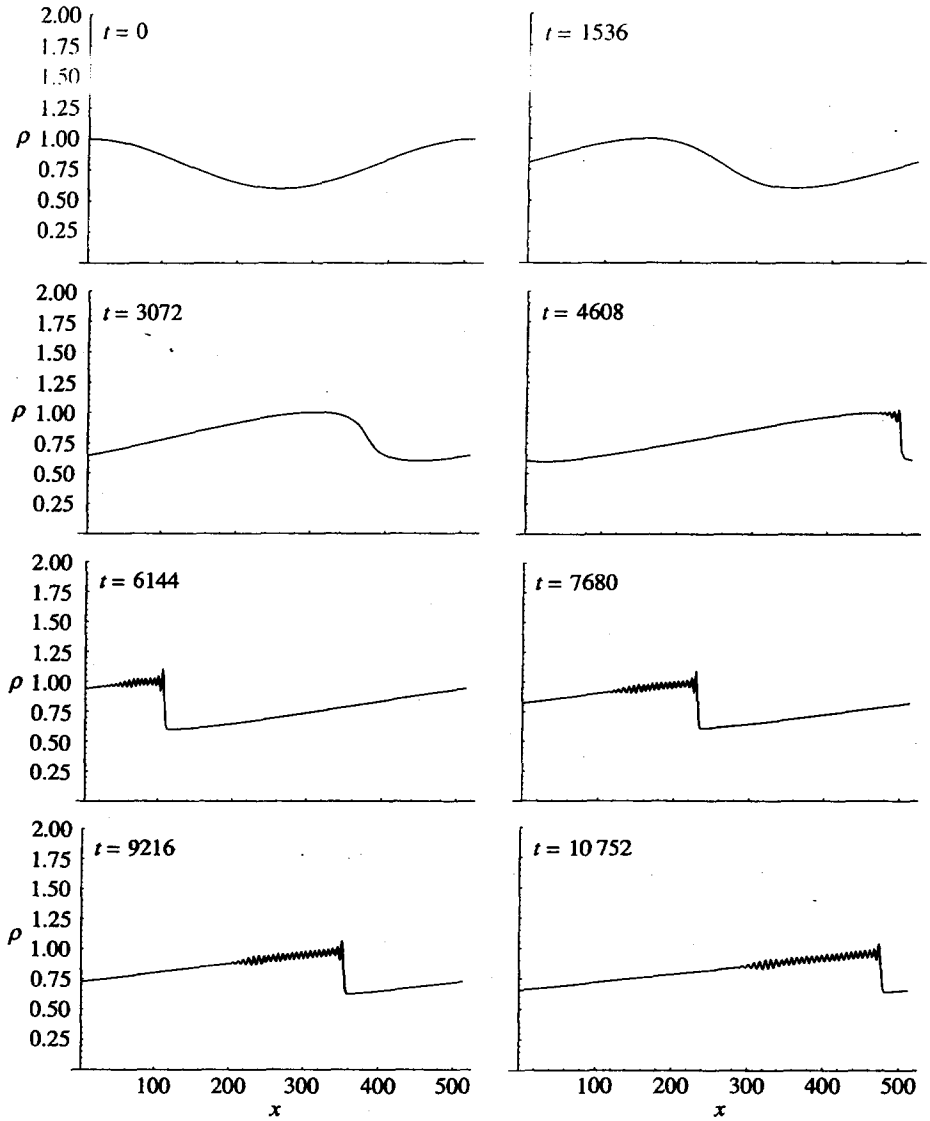

Figure 3. $\rho(x,t)$ versus x for a sequence of times t for $N = 512$ and $\kappa = 0.01$.

turbulent relaxation at finer scales is captured by the change in a suitably defined Lyapunov function. Thus, entropic models used for this purpose may likewise be susceptible to oscillations and other parasitic dynamics which, though bounded in amplitude and scaling to zero in the continuum limit, may seriously undermine efforts to use the model for the accurate quantitative study of turbulence.

Having said the above, we stop short of suggesting that these oscillations preclude the use of entropic collision operators for subgrid studies of turbulence. To some extent, the tests that we have conducted in this paper are unduly stringent: we have noted inaccuracies in the evolution of the model for one particular set of initial

conditions. Most subgrid models endeavour to achieve quantitative faithfulness only to quantities that can be averaged robustly over ensembles of various sorts. For this purpose, inaccuracies in any one instantiation may be unimportant as long as they do not affect the ensemble average. Thus, a better test would be the use of the model described herein to simulate Burgers's turbulence over an ensemble of initial conditions on ever coarser grids. We leave this matter to future work.

P.J.L. was supported by the DARPA QuIST program under AFOSR grant number F49620-01-1-0566. B.M.B. was supported in part by the US Air Force Office of Scientific Research under grant number F49620-01-1-0385, and in part by MesoSoft Corporation; he also acknowledges the hospitality of the Centre for Computational Science at University College London, where some of this work was carried out under the EPSRC's RealityGrid programme. Finally, B.M.B. is grateful to Sauro Succi for helpful conversations.

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